Used Fuel Disposition Campaign

Process Modeling and Investigations For Clay/Shale Repositories: Natural Barrier System

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FY13 Work Activities

- **THMC Model Capabilities for Clay Repositories**
  - *Coupled Thermal-Hydrological-Mechanical (THM) Discrete Fracture Model (DFM) for Argillaceous Rock, Including Fracture Propagation (Asahina/Houseworth/Birkholzer)*
  - *Constitutive relationships and HM Modeling of the Mine-by Test at Mont Terri (Liu/Li/Birkholzer)*

- **Thermal Limit Testing**
  - *High Temperature Laboratory Experiments (Nakagawa/Kneafsey/Ajo-Franklin/Birkholzer)*
  - *Detailed Mechanistic Modeling of THMC Alterations (Zheng/Finsterle/Birkholzer)*
  - *Impact of High-Temperature THMC Changes on Radionuclide Transport and Other PA drivers (Finsterle/Zheng/Birkholzer)*

- **Radionuclide Interaction and Transport in Representative Geologic Environments**
  - *Modeling Radionuclide Interaction and Transport in Clay Formations (Zheng)*

FY13 Work Activities

- **Modeling hydrologic flows in representative geologic media**
  - *Investigation of Non-Darcy Flow Behavior in Clay (Liu/Li/Birkholzer)*

- **International Collaborations**
  - *THM Modeling of FE Heater test at Mont Terri URL (Rutqvist/Chen/Birkholzer)*
  - *Discrete Fracture Interpretation of the HG-A Test at Mont Terri (Asahina/Houseworth/Birkholzer)*

- **Deliverables**
  - Level 2 - *THMC modeling of the near field evolution of a generic clay repository: Model validation and demonstration* (08/15/2013)
  - Level 4 - *Report on THMC effects on radionuclide transport in a clay repository* (8/15/13)
  - Level 4 - *Report on hydrologic flows in low permeability media* (11/13/13)
  - Level 4 - *Report on international collaborations on FE heater and HG-A tests* (11/6/13)

Major FY12 Accomplishments

- The two-part Hooke's model (TPHM) was implemented into the TOUGH-FLAC3D code and tested against data from the Mine-by Test at Mont Terri URL.
- A new three-dimensional DFN modeling tool for coupled flow and geomechanical processes, capable of addressing fracture initiation and propagation, was developed.
- Preliminary TH and THM model simulations of the FE test at the Mont Terri URL were performed for the purpose of validating modeling capabilities for THM processes.
- The TOUGHREACT-FLAC3D (THMC) simulator was further enhanced and used for a preliminary evaluation of the THMC impact on radionuclide transport processes.

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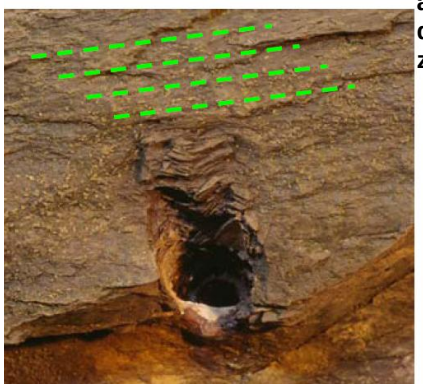
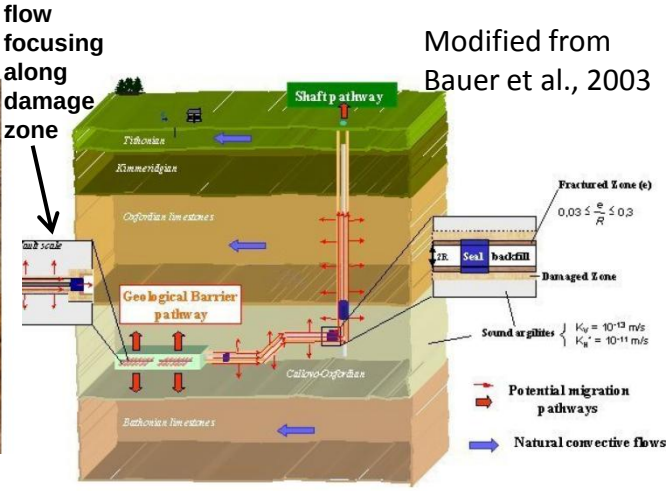
Coupled Thermal-Hydrological-Mechanical (THM) Discrete Fracture Model (DFM) for Argillaceous Rock

- **Argillaceous formations that may be available for nuclear waste disposal are typically saturated**
  - Suitability of argillaceous rock rests in large part on an effective and robust low-permeability attribute
- **Fracturing is the most likely threat to the low-permeability attribute of an argillaceous rock:**
  - Repository-induced THMC disturbances cause fracturing along repository openings
  - Natural disturbances (e.g., abnormal pressure – induced hydrofractures) cause fracturing at the formation scale
- **Fractures in argillaceous rock tend to be short-lived because of self-sealing behavior**
  - Can lead to poorly-connected fractures during fracturing episode
  - Potential fracture-matrix cross-flow interaction
  - Coupled process DFMs more representative

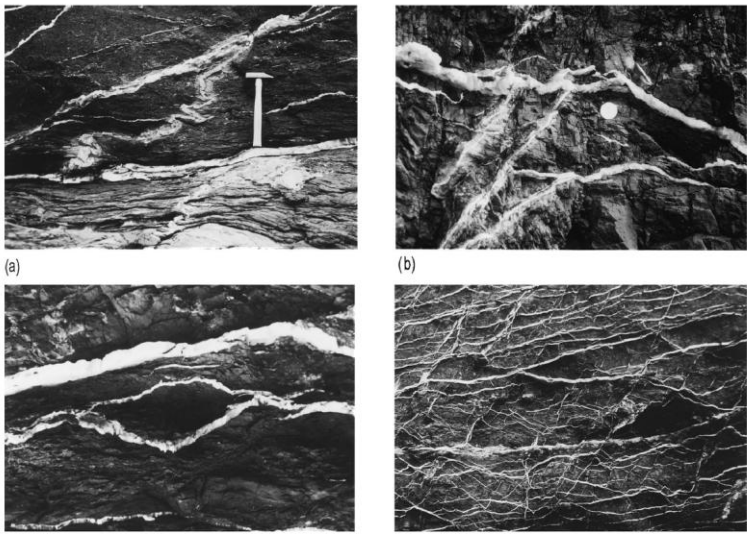
Blümling et al., 2007



Modified from Bauer et al., 2003



Mercia Mudstone, Bristol Channel Basin, UK: natural hydraulic fractures filled with sand and gypsum



Cosgrove, 2001

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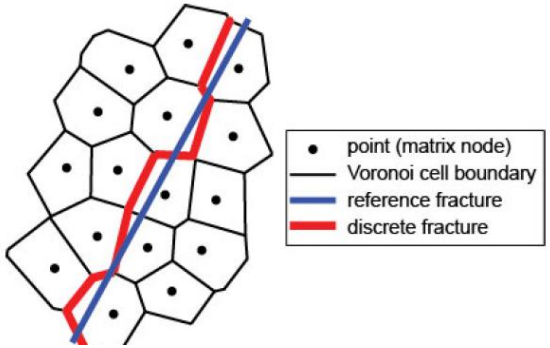
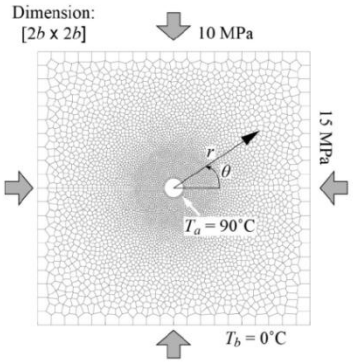
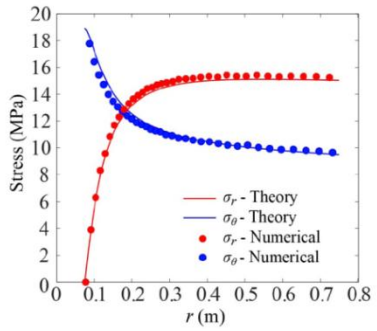
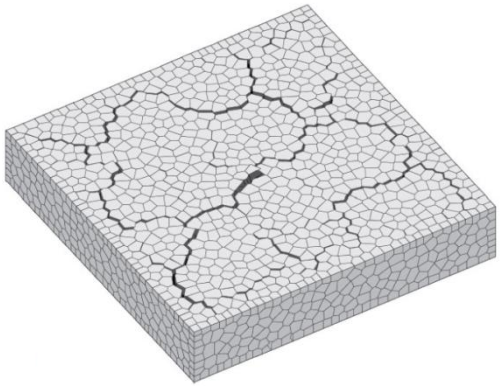
Coupled Thermal-Hydrological-Mechanical (THM) Discrete Fracture Model (DFM) for Argillaceous Rock

- **THM dynamic fracturing model based on coupling TOUGH2 thermal-hydrological model with Rigid-Body-Spring Network (RBSN) geomechanical fracture-damage model**
  - Both operate on same Voronoi grid; fractures are mapped onto edges of Voronoi cells
  - Flow /transport and coupled HM /TM processes have been analyzed and compared with analytical models or alternative numerical models
  - Fracture initiation and propagation coupled with hydrologic model has been analyzed for problem of desiccation-induced fracturing
- **FY13 work activities**
  - Validate desiccation-induced fracturing model against experimental data from literature
  - Implement coupling for
    - strain effects on porosity, permeability
    - fluid pressure-geomechanics for hydraulic fracturing
  - Evaluate repository-induced and natural fracturing, more complex fracture networks, and self-sealing
  - Conduct HG-A modeling (see international collaboration)









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Constitutive Relationships and HM Modeling of the Mine-by Test at Mont Terri

❑ Objective

Constitutive relationships are key elements for modeling coupled processes. The major objective is to develop and validate the relationships for clay rock.

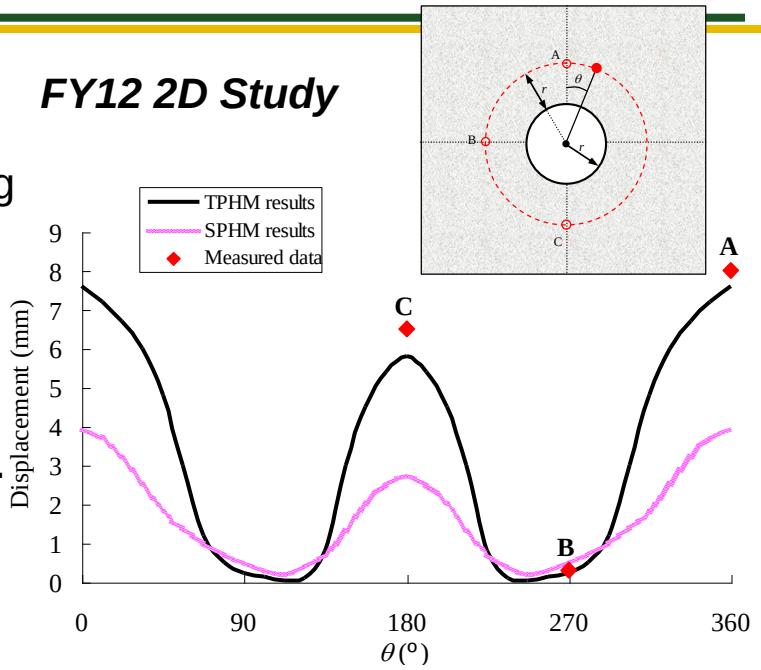
❑ Approach

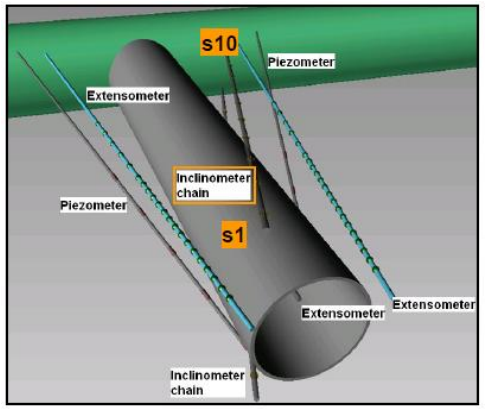
Based on two-part Hook's model and TOUGH2-Flac3D.

❑ FY13 Work

- FY12 work is a preliminary 2D study that cannot capture all the important features of the Mine-by test at Mont Terri. A 3D model will be developed in FY13 to incorporate all the events in the test.
- Modeling results will be compared with available data from the Mine-by test including displacement and pore pressure as a function of time.

FY12 2D Study





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Thermal Limit Testing:
High Temperature Laboratory Experiments

Objective:

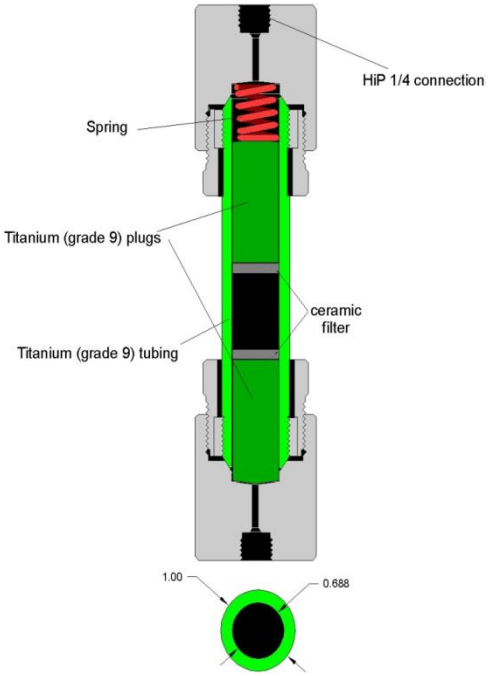
Investigate the impact of heat-induced chemical alterations (smectite-to-illite transformation) of buffer and backfill materials (bentonite) and clay host rock on their geomechanical and hydrological properties (mechanical strength, permeability, seismic velocity)

Approach

- Test bentonite clay with a range of (1) porosity (density), (2) water content (below saturation), (3) KCl concentration
- Multiple samples are heated (from 100°C to 300°C) in sealed, spring-loaded cylindrical titanium miniature pressure vessels
- Changes in volume, acoustic velocity, permeability, and mechanical strength are examined for different heating durations
- Chemical/mineral testing in collaboration with LANL
- Integration with modeling work (TOUGHREACT-FLAC3D)

FY2013 Work

- Fabrication of miniature pressure vessels
- Preparation of experimental system
- Acquisition and baseline characterization of clay samples
- Preliminary experiments for verifying system performance



Miniature pressure vessel ("test tube")

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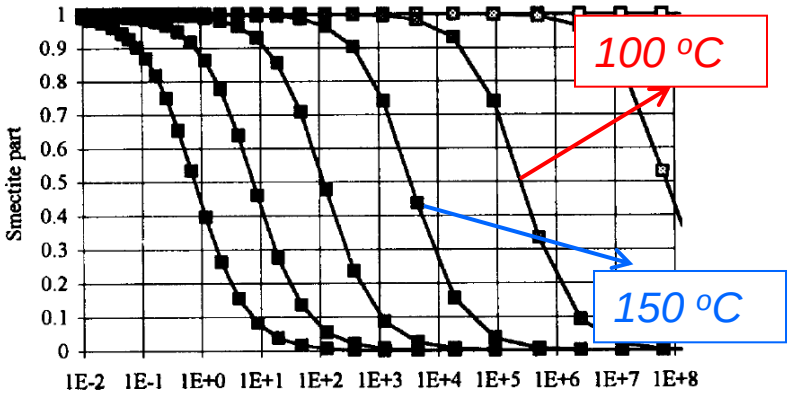
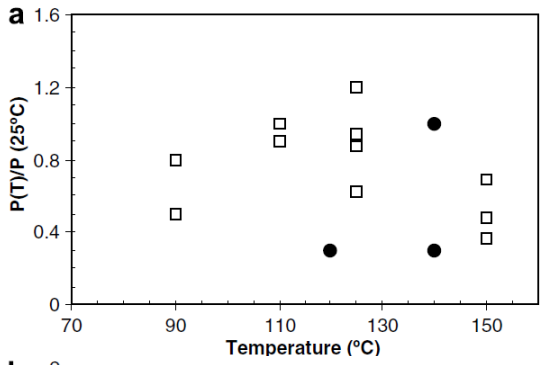
Thermal Limit Testing:

Detailed Mechanistic Modeling of THMC Alterations

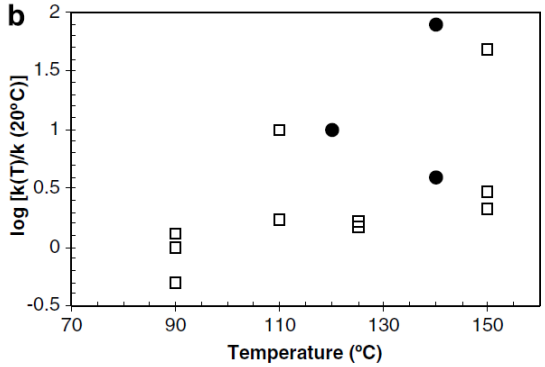
Motivation

- Illitization, the transformation of smectite to illite, results in a loss of swelling capability of EBS and clay host rock.
- The rate of illitization increases as temperature increases, with about two orders of increase if temperature increase from 100 to 150 ^{o}C according to a theoretical model .
- However, many factors such as the availability of potassium, proton and water constrain the illitization. A model that could consider all the relevant factors is needed to evaluate the illitization in EBS and clay host rock.
- The mechanical and hydraulic consequences of illitization also need to be evaluated.





Swelling pressure



Hydraulic conductivity

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Thermal Limit Testing:

Detailed Mechanistic Modeling of THMC Alterations

Objective:

Evaluating the degree of illitization in EBS and clay host rock under high temperature (100 to 200 ^{o}C) conditions and the subsequent effects on the mechanical and hydraulic properties of EBS and clay host rock

- **Approach**
  - Detailed mechanistic modeling with TOUGHREACT and TOUGHREACT-FLAC3D

- **FY2013 Work**
  - Establishing the geochemical conceptual model based on detailed understanding of the reaction network of illitization under typical clay repository environment.
  - Developing a THC model to evaluate the degree of illitization in EBS and clay host rock for temperature from 100 to 200 ^{o}C under different geochemical and hydraulic conditions.
  - Developing coupled THMC model to assess the swelling pressure and hydraulic conductivity changes as a consequence of illitization

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Thermal Limit Testing:

Impact of High-Temperature THMC Changes on Radionuclide Transport and Other PA drivers

Objective:

Develop modeling methodology supporting PA of a high-temperature repository

Design and optimization of high-temperature repository

- **Approach**
  - Identify high-temperature scenarios and related effects (see previous task)
  - Determine method to include THMC effects in system-level models
    - Coupled process models
    - Empirical correlations
    - Reduced-order modeling
  - Define performance measures to be used for analysis
  - Develop simulation and uncertainty quantification methodology for evaluation of (potentially correlated) scenarios and parameter cases
  - Determine scenarios and parameters with significant influence on high-temeprature repository performance
  - Outline future analysis and optimization studies

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Modeling Radionuclide Interactions and Transport in Clay Formations

Objective:

Modeling radionuclide reactive transport in clay formation with a focus on using data from other labs for surface complexation model improvement and further enhancing the THMC modeling capability

- **Approach**
  - Detailed mechanistic modeling with TOUGHREACT
- **FY2013 Work**
  - Building surface complexation reaction network based on experimental data for U and Pu sorption on clays and iron hydroxidizes from UFD (e.g. U sorption study at LBNL or Pu sorption study at LLNL) and other sources. If possible, compile these reactions into a consistent database
  - Incorporating temperature effect into surface complexation reactions and testing them with available data
  - Developing a THC model to evaluate the migration of U and Pu in clay formation under different geochemical and hydraulic conditions
  - Implementing more constitutive mechanical-chemical coupling relations such as linking BExM (Barcelona Expansive Model) with chemical reactions to enhance our capability of simulating THMC processes

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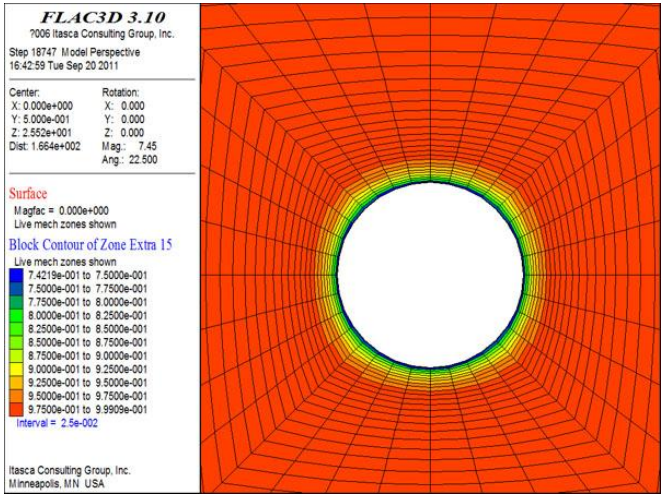
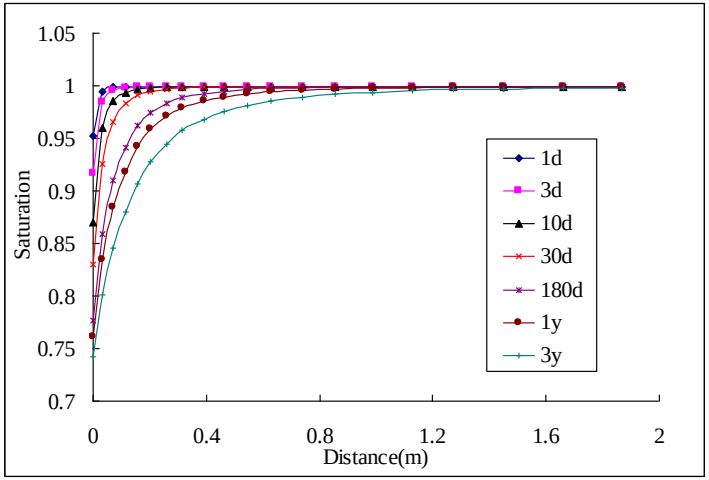
Investigation of Non-Darcy Flow Behavior in Clay

Importance of non-Darcy flow in clay

- Excavation Damaged Zone (EDZ) is a critical feature impacting repository performance.
- Desaturation and resaturation are important for EDZ evolution (shrinkage-induced fracture; fracture self-sealing).
- Water flow from host rock to EBS is critical for buffer to function (swelling).





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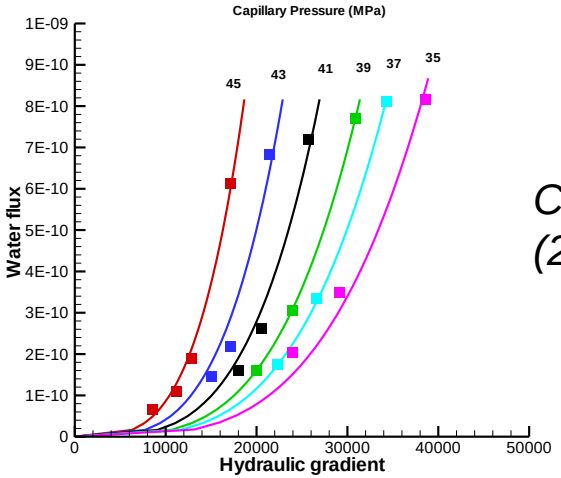
Investigation of Non-Darcy Flow Behavior in Clay

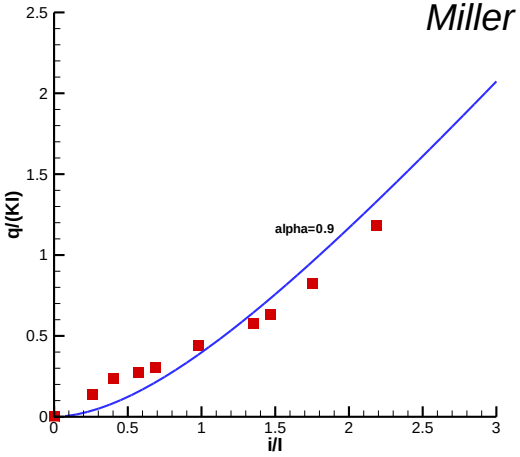
Approach and FY13 Work Scope

- Development of approach to incorporate temperature impact based on data from petroleum literature.
- Development of a modeling capability for non-Darcy flow by incorporating FY12 development into TOUGH2 code.
- Integration with LANL's neutron-scattering test results.



Cui et al. (2008)

Miller and Low (1963)



International Collaborations: THM Modeling of FE Heater Test at Mont Terri URL

Objective:

In situ investigations and model validation related to repository induced coupled thermo-hydro-mechanical (THM) processes and their effect on the host rock

Approach

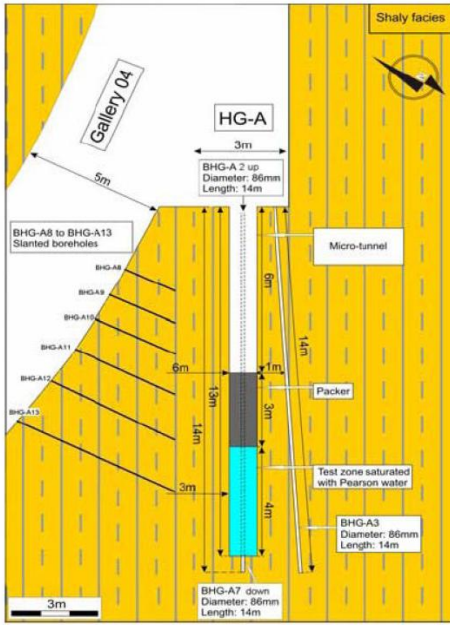
- TOUGH-FLAC simulator using layered (anisotropic) rock mass THM model of Opalinus Clay and Barcelona Basic Model (BBM) for bentonite THM behavior.

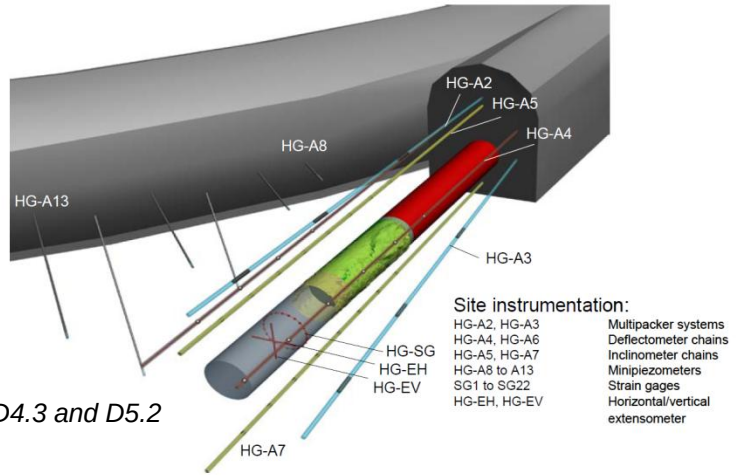
FY2013 Work

- Develop a 3D TOUGH-FLAC model (grid) of the FE Heater test based on current preliminary 2D model.
- Conduct modeling of laboratory THM experiments for parameterization of BBM material parameters related to granular bentonite buffer materials.
- Modeling of FE tunnel excavation with comparison to measured rock mass responses when data available.
- 3D model predictions of THM evolution during heating test

International Collaborations: Discrete Fracture Interpretation of the HG-A Test at Mont Terri

- **The HG-A test is being conducted at the Mont Terri URL**
  - HG-A microtunnel is 13 m long, 1 m in diameter
  - array of instrumented boreholes measuring stress, strain, fluid pressure, and water content during water and gas injection
- **The test is focused on:**
  - conceptual understanding of damage zones around cylindrical excavations
  - hydraulic conductivity of the Opalinus Clay on the tunnel scale
  - self-sealing processes along the damage zones around backfilled tunnels
  - gas leakage rates from sealed tunnel sections
- **For FY13, the coupled THM-DFM will be used to examine test data and interpret EDZ**
  - disturbed zone fracturing
  - hydraulic behavior
  - fluid-displacement processes
  - fracture self-sealing





FORGE Report D4.3 and D5.2 – VER 1.0 , 2010